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Report on CCP13 Software Developments: Production of an Integrated CCP13 Environment (ICE) for Windows

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ABSTRACT

*We report on recent developments in CCP13 software with particular emphasis on **ICE**, an integrated, internet-enabled, common desktop CCP13 environment. As an initial package, several heavily used data conversion and stripping programs have been integrated together in **ICE** with an easy to use Graphical User Interface (GUI) and enhanced functionality. **ICE** can dynamically group CCP13 programs together by using a program startup panel. At present the programs that have been integrated with **ICE** include CCP13 **ImageViewer**, XCONV, FTOREC, LSQINT, XFIX and the CCP13 **Online Help** Browser.*

Introduction

One of the main goals of CCP13 is to develop software for non-crystalline diffraction. Over the last ten years CCP13 scientists have been developing and supporting a set of programs for stripping and analysing fibre diffraction patterns and other non-crystalline diffraction patterns and for systematic modelling of different kinds of structure. CCP13 software has become one of the important shared resources for the fibre diffraction, non-crystalline diffraction and solution scattering research community in the UK and world-wide. The aim of the CCP13 project has been to allow geographically distributed research groups to work together more effectively, sharing resources, data, knowledge and expertise in the community and to allow those multi-discipline groups to complete their tasks quickly and smoothly. Several recent developments as part of the CCP13 project have helped to promote these ideas, including providing an active CCP13 website and its mirror sites, providing updated and newly developed software for download, and providing the online version of *Fibre Diffraction Review*. Here we describe the recent development of the integrated CCP13 environment software known as ***ICE***.

Recent Developments for Fibre Diffraction

A major task for the CCP13 effort has concerned the extraction of useful intensity data from fibre diffraction patterns. The nature of the patterns from fibres can be quite diverse, ranging from those which exhibit Bragg sampling from polycrystalline specimens, to patterns where the intensity is continuously distributed along layer-lines, reflecting a complete lack of axial register across the sample. As a first attempt at providing an integrated software package, several heavily used data conversion and stripping programs have been put together into a user-friendly package with an easy to use Graphical User Interface (GUI) and enhanced functionality. This package is now called ***ICE***. Users can still enjoy the freedom to start up and use each individual program independently by opening them either from the program menu or from the ***ICE*** common desktop environment.

ICE is an integrated, internet-enabled, common desktop CCP13 environment. It can dynamically group the CCP13 programs together by using a program start-up panel. In ***ICE*** version 1.0, six applications have been developed and integrated. They are: CCP13 ***ImageViewer***, XCONV, FTOREC, LSQINT, XFIX and the CCP13 ***Online Help*** Browser. ***ICE*** also provides a CCP13 program editor so that users can use it to create batch files for applications like FTOREC and LSQINT in order to run them under the batch mode. Like any integrated commercial program editor, it supports functions such as copy, cut, paste, print, font and colour selection. The motivation to do this is that the user has to conduct a sequence of related computational tasks quite often and repeatedly. Such tasks flow from one application (e.g. XCONV) to a second application (e.g. XFIX) and so on. This is a 'work flow' problem and is very common in CCP13 processing, as described in Squire *et al*. (2003). For instance, to process a raw fibre diffraction pattern, the raw data can be viewed initially by ***ImageViewer***. Then it is put through the file conversion program XCONV to convert it into BSL format and the BSL image may itself be displayed and manipulated by ***ImageViewer***. The BSL image is then put into the analysis program XFIX which outputs parameters such as fibre tilt and rotation for input into FTOREC, where the pattern is corrected and remapped into reciprocal space. Then, the corrected data from FTOREC can be fitted in LSQINT either as continuous intensities or as Bragg peaks after suitable background removal. Intensities output from LSQINT can then be used in modelling processes. The philosophy behind the development of ***ICE*** is to make possible a much improved pattern of 'work flow' through these CCP13 programs. ***ICE*** is an XML-enabled environment. XML can play a key role as a data definition language in the 'work flow' problem when transferring data from one application to another. To make implementation of a sequence of related computational tasks both quick and reliable, it is possible to use the integrated program editor to support the syntax and grammar checks for creating batch files and work flow files. Using 'drag and drop' to view images and texts has become a standard feature in the ***ICE***-enabled applications.

ICE consists of a menu bar, a tool bar, a program startup panel and a CCP13 program text editor as presented in Figure 1.

Both ***ImageViewer*** and ***Online Help*** are newly developed CCP13 applications. CCP13 ***ImageViewer*** intends to provide comprehensive visualisation and image data manipulation capability. It will be used to preview different types of images before running XCONV and will be able, for example, to rotate the images in a series through a defined angle to align them parallel to a common axis, to scale them to a common size, and to put them on a common centre, so that several images can be added to increase the signal to noise. CCP13 ***Online Help*** provides specific online help and support to the CCP13 users, powered by the newly developed internet-enabled CCP13 web browser which makes automatic online updates of the ***ICE*** software and documents possible. The tool bar of ***ICE*** includes

XFIX is designed to help ascertain some important parameters of a fibre diffraction pattern. Information such as the pattern centre, detector orientation and fibre tilt can be estimated and refined and putative unit cells can be plotted over the pattern. In addition, more general functions are available such as the capability to plot and fit integrated slices or scans through the pattern. The program can also be used to remove the background of fibre diffraction patterns. XFIX has been newly designed and developed for Windows. This has improved the application's stability, expandability, modularity and performance. It has replaced the original loose-coupled communication between XFIX and the background FIX application with one application that combines both BSL image

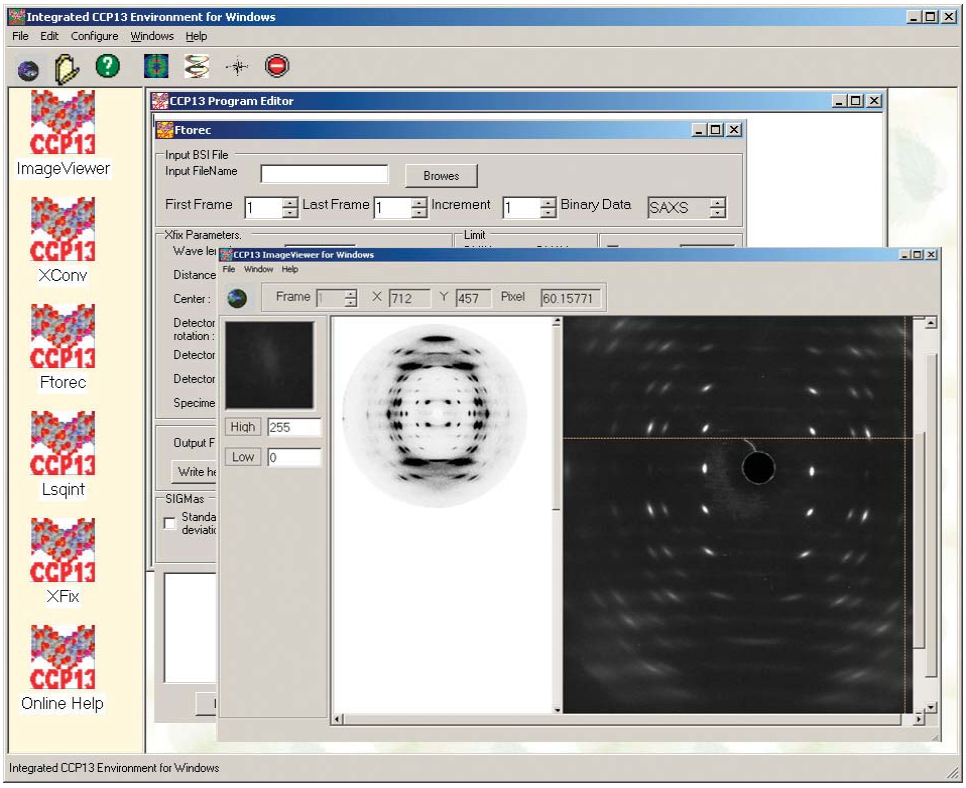

Figure 1. The Integrated CCP13 Environment (*ICE*) for Windows, showing opened FTOREC and ImageViewer windows.

speed image buttons so that users can start a Microsoft file explorer, access the CCP13 ***Online Help***, CCP13 website and *Fibre Diffraction Review* website directly by using the CCP13 web browser. The reason for including Microsoft File Explorer is that 'Drag and Drop' functionality is supported by most of the ***ICE***-enabled applications such as XFIX and ***ImageViewer***. For example, you can drag a JPG image file from Microsoft File Explorer and then drop it onto CCP13 ***ImageViewer*** to be displayed. Furthermore, most of the ***ICE*** integrated applications support hint-tip style text sensitive help when your mouse is over a command button. XCONV, FTOREC, LSQINT and XFIX have been ported from UNIX to Windows with enhanced functionalities.

XCONV is a program that can input data files from a variety of data sources and can convert them to BSL/TIFF formats. BSL format is at present the standard format for most of the CCP13 processing software. XCONV has been newly developed under Microsoft Windows with enhanced support for a wide range of image file formats from a variety of detectors and will be continuously updated as new detectors and image formats are used. The newly supported image formats include Mar345, BRUKER and ILL_SANS. Please refer to the ***Online Help*** document for details.

display and data-processing functions together. Plotting and fitting integrated slices or scans through the pattern was supported by the original version of XFIX by using third party graphical image display software PGPLOT. The current version of XFIX has replaced this by introducing our own CCP13 image display modules with enhanced visualisation capability and extendibility. Background subtraction and refinement in XFIX was always a time-consuming process. The computational speed has now greatly improved. The new version of the XFIX drawing objects function is quite easy to use as well. Furthermore XFIX can now handle any size of image. Since FTOREC is integrated with XFIX, it automatically passes the parameters that need to go to FTOREC. The postscript format output in the original XFIX has been replaced with JPG and BMP image formats.

FTOREC is designed to take all or part of a diffraction image and to transform this portion of the image into reciprocal space, given knowledge of the specimen to film distance, orientation of the image, wavelength and tilt of the specimen determined in XFIX. FTOREC has been re-developed under the Microsoft .Net platform as a user-friendly GUI application. It can run under ***ICE*** as a standalone application and it has also been integrated into a part of XFIX as well. LSQINT provides an

automatic method for the integration of intensities for fibre diffraction data. It has been newly developed and supports three modes: the non-GUI DOS command line mode, the batch Windows mode, and the Windows GUI mode.

Future Developments

Feedback from users has suggested that there is still plenty of room for further improvements to the ***ICE*** software and that we should also develop and integrate more CCP13 applications into ***ICE***. In fact, instrumentation and experimentation developments are already pushing for improvements in existing CCP13 programs. For example, where high spatial precision is needed in X-ray diffraction patterns, A3 size image plates are being used with a pixel size of about 100mm. This generates enormously large files. The lack of standardisation of file formats and the increasing number of new detectors and raw image data formats are also pushing for continuously updating inter-conversion programs such as XCONV. There are also increasing demands for visualising and pre-viewing the raw images in the new data formats.

LSQINT can handle patterns which are largely crystalline in nature, or patterns which have intensity continuously distributed along layer-lines, with sampling only occurring parallel to the c-axis. More than one lattice can be fitted in a single pattern. The approach used is to generate spot profiles and then to fit these profiles to the observed pixel values. The current version of LSQINT for Windows is a GUI-based application supported by the LSQINT DOS application in the background. Running the LSQINT program is a time-consuming process. Planned improvements will include shorter processing times, improved data visualisation and display and a more user-friendly GUI, as well as removal of the restrictions on the dimensional size of an input image.

The subtraction of appropriate backgrounds plays an important role in extracting high quality data from fibre diffraction patterns. In LSQINT and XFIX, several background subtraction methods are available. For example, a global background can be fitted simultaneously with the spot profiles; a notional roving aperture and filter can be used to define a background; or a background plane can be fitted in a region of the pattern along with the spot profiles. The on-going tasks include the development of better background subtraction modules, the design and development of new background subtraction algorithms, the further reduction in background subtraction and refinement processing time, and the implementation of these modules in both XFIX and LSQINT.

On the other hand, the existing CCP13 software, now proved and accepted as being effective and robust, needs to be made as simple to handle as possible for new users. Many users are currently trying out the CCP13 software for their own applications. This is both testing the software under varied real world conditions and also, in some cases, leading to requests for the software to be modified or enhanced for user specific needs. There remains a major task of improving user interfacing; specifically in the writing of up-to-the minute, comprehensive and comprehensible manuals for the various software packages, including self-help tutorials.

Conclusions

Traditionally, CCP13 software has been developed and supported under various UNIX platforms, and UNIX Workstations have been the main computational resources for fibre diffraction researchers. However, this situation is changing. Upgrading and maintaining UNIX workstations is more expensive than for PCs, and, because of the growth in computer speed, disk capacity and memory, modern PC workstations running under Linux or Microsoft Windows can be very powerful machines in their own right. During the past decade, Linux has had a large impact on the traditional UNIX platforms, and major UNIX machine providers such as Sun, IBM and HP have run to support Linux as well. There have been very useful developments in the implementation of CCP13 packages on Linux which can reside either on Intel-powered relatively inexpensive PCs or on traditional UNIX workstations. However, Linux may not be available free of charge in the near future as SCO is demanding Linux license payments. The potential impact of this on academic users is not clear. On the other hand, the Microsoft Windows operating system and software development toolkit have now become almost free for academic use under Microsoft campus agreements. This enables us to develop and to maintain high standard user-friendly graphical user interface (GUI) and visualisation applications across Windows platforms. CCP13 programs need to support visualisation, frequent user and program interaction, and time-consuming tasks as well. Nowadays, most of the CCP13 users have a PC, but they have lacked a set of CCP13 programs running under Windows. Following the successful porting of CCP13 programs into DOS, several of the most widely used CCP13 applications have now been developed under the Microsoft Windows environment to support the majority users of PCs. For example, ***ICE*** is a software package intending to make CCP13 software as readily, extensively and productively used as possible. It will meet demanding tasks such as those of both high computational performance and graphic visualisation capacity and, at the same time, it is hoped that it will reduce the "energy barrier" for new users as well as providing additional useful functionality. One of the on-going tasks for the forthcoming months is to deliver ***ICE*** for Linux. Both Linux and Windows have large user bases in our community. It is important to deliver solutions for both operating systems.

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